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Title:	Physics-Informed Machine Learning for Discovery and Optimization of Materials: A Case Study of Scintillators
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Physics-Informed Machine Learning for Discovery and Optimization of Materials: A Case Study of Scintillators

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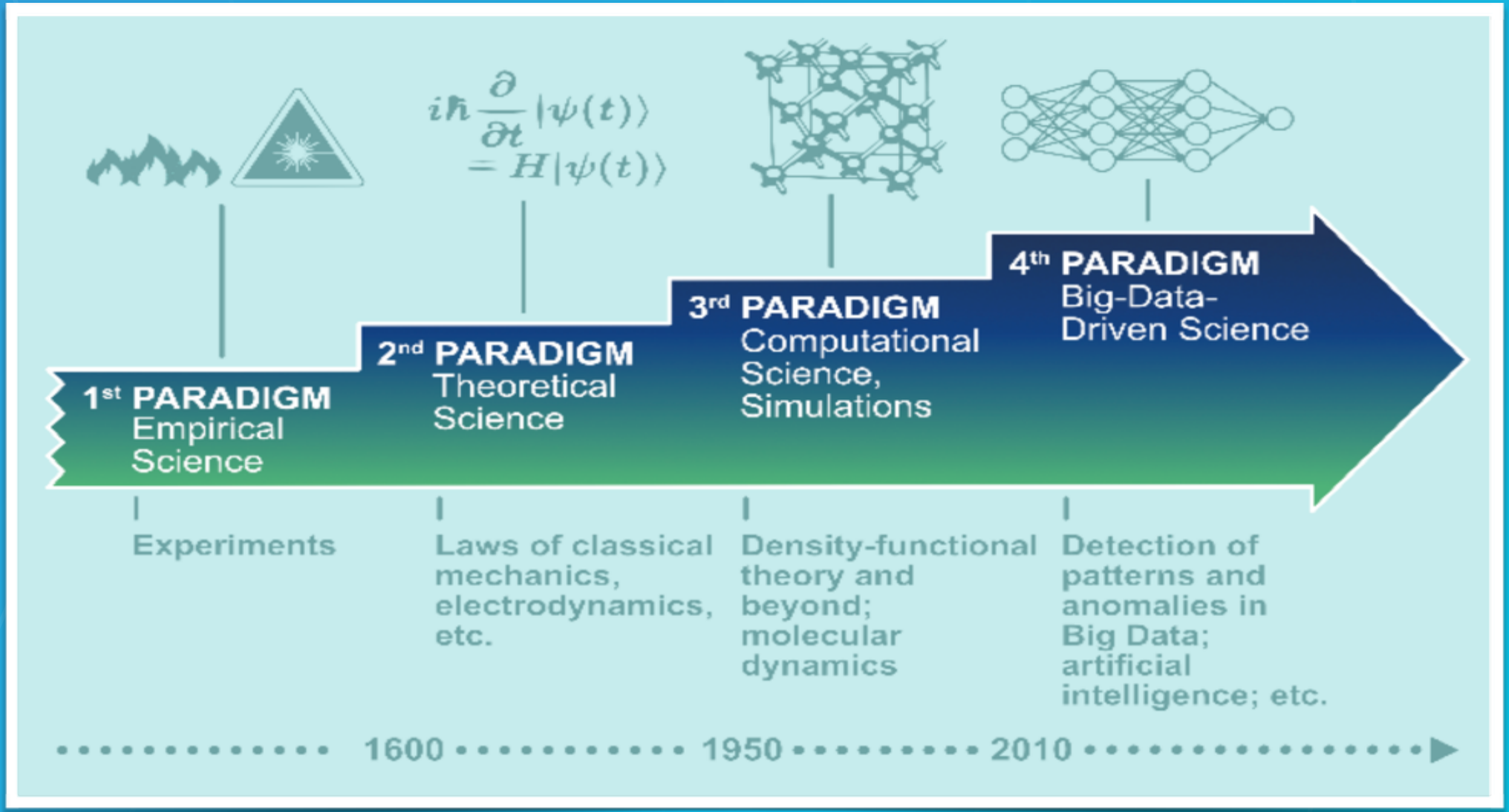
- Data-enabled design as a fourth paradigm in materials science
- Physics agnostic v/s physics informed machine learning (ML)
- Can we find new materials or optimize existing ones using ML?

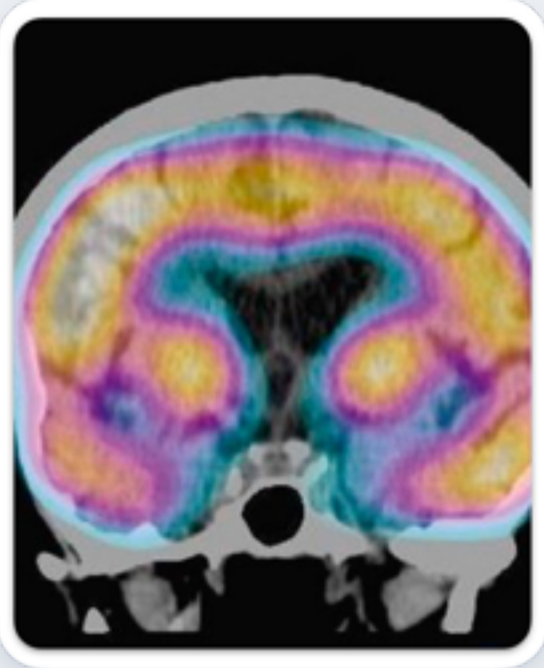


C. Draxl, M. Scheffler, NOMAD: The FAIR Concept for Big-Data-Driven Materials Science (2018), R Ramprasad et al. Machine learning in materials informatics: recent applications and prospects, NPJ Comp. Mater. 3, 54 (2017).

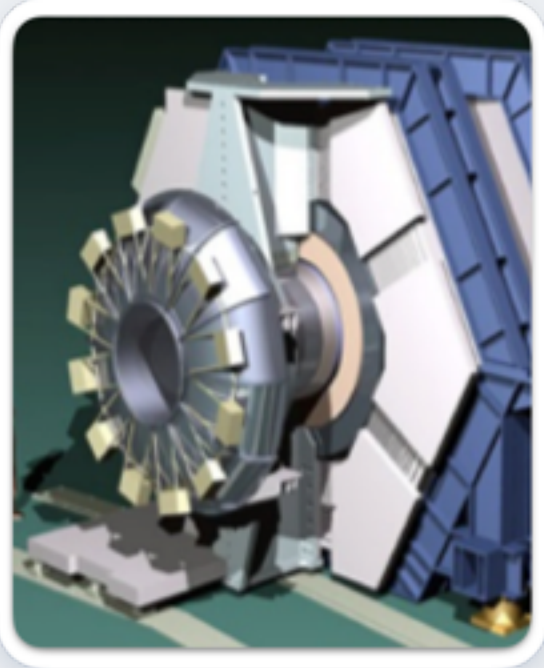
University Outreach Workshop
Wednesday August 1, 2018, MSL Auditorium

Discovery and Design of Novel Scintillators

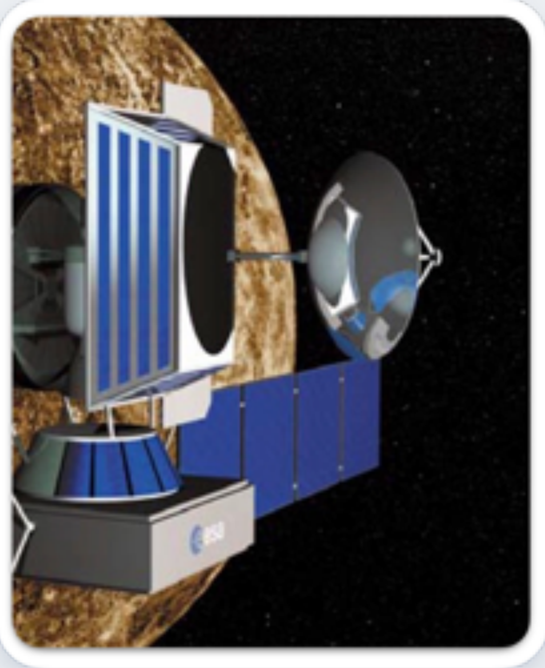
Global Security
& Threat Reduction



Medical Imaging

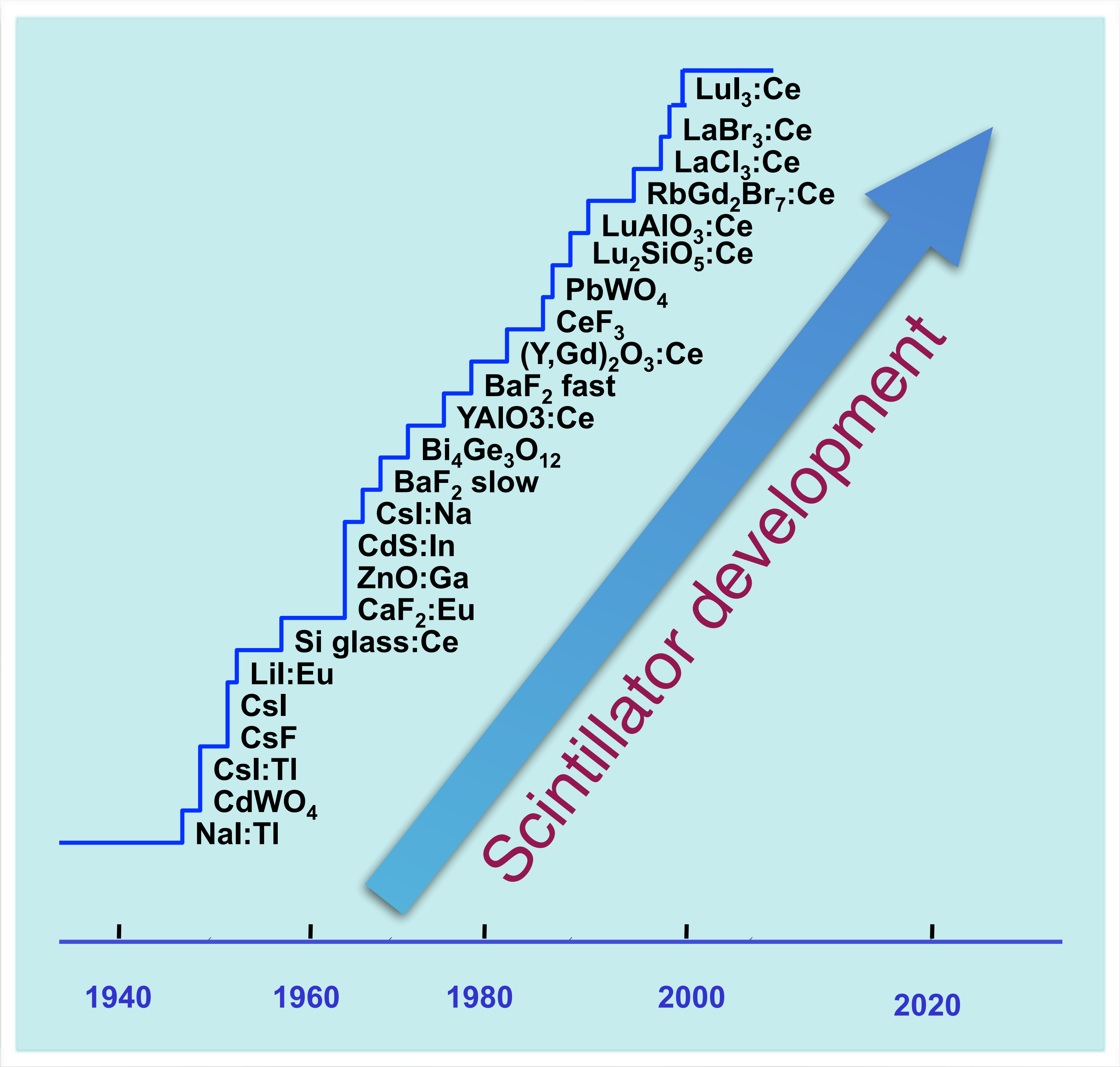


High Energy Physics
Experiments

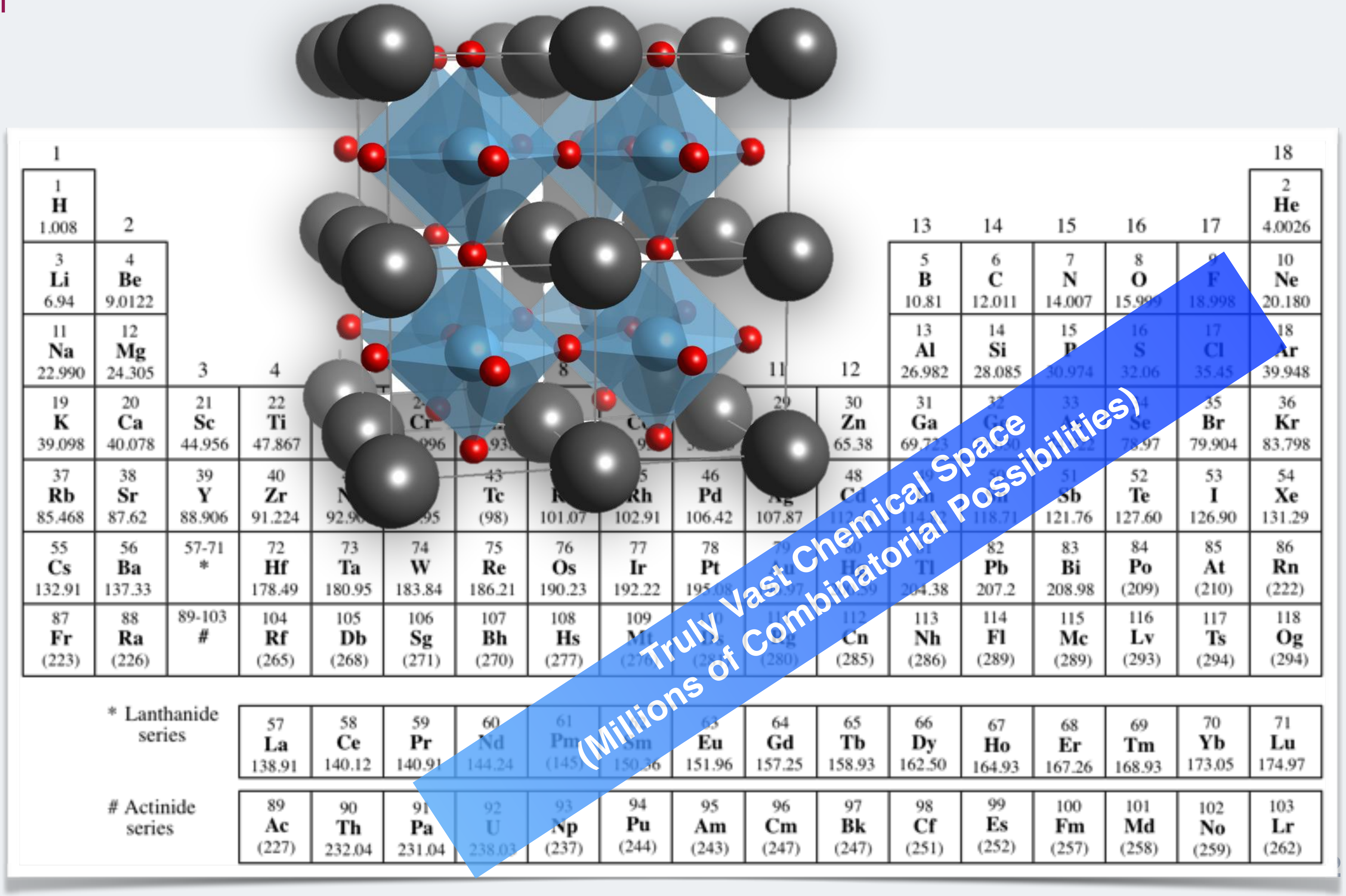


Space Research

Radiation detector materials — including scintillators — are also critical to a number of applications as well as existing and upcoming experimental facilities of direct interest to LANL, *e.g.*, ECSE, MaRIE and p-RAD.



Scintillator discovery and development has largely been guided by chemical intuition and laborious trial-and-error based experimentation.

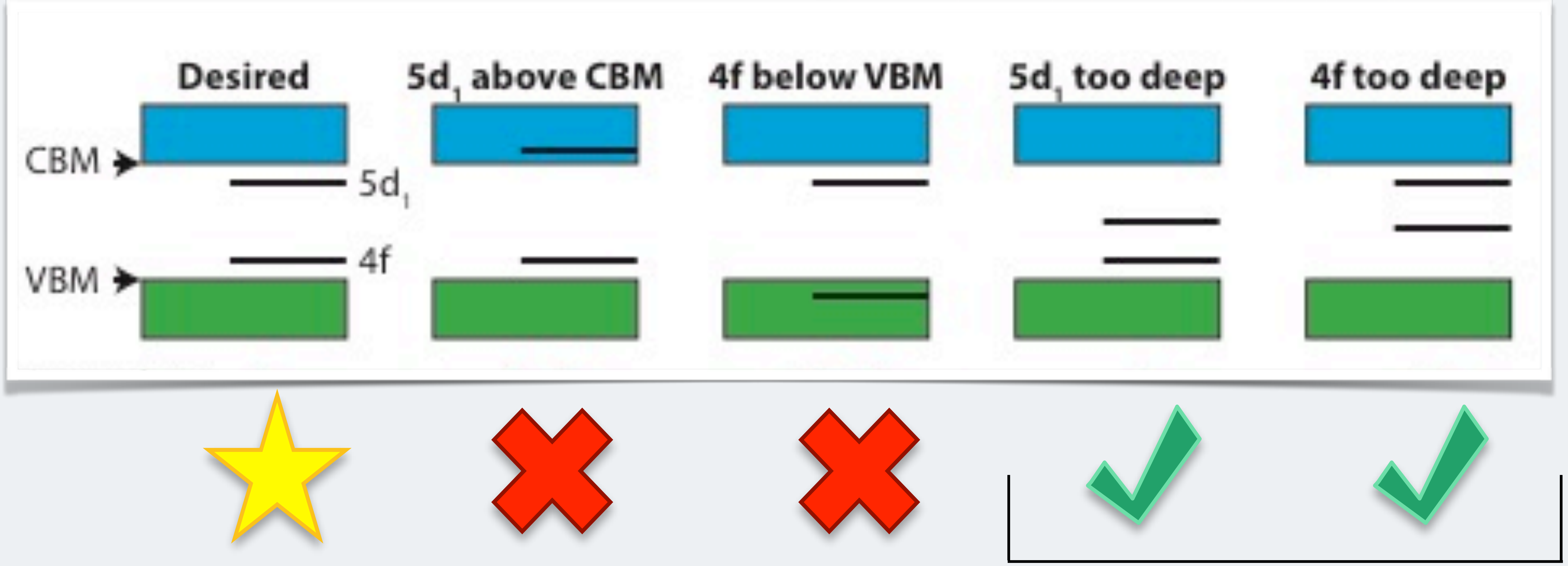


Scintillator *versus* Non-Scintillator Screening

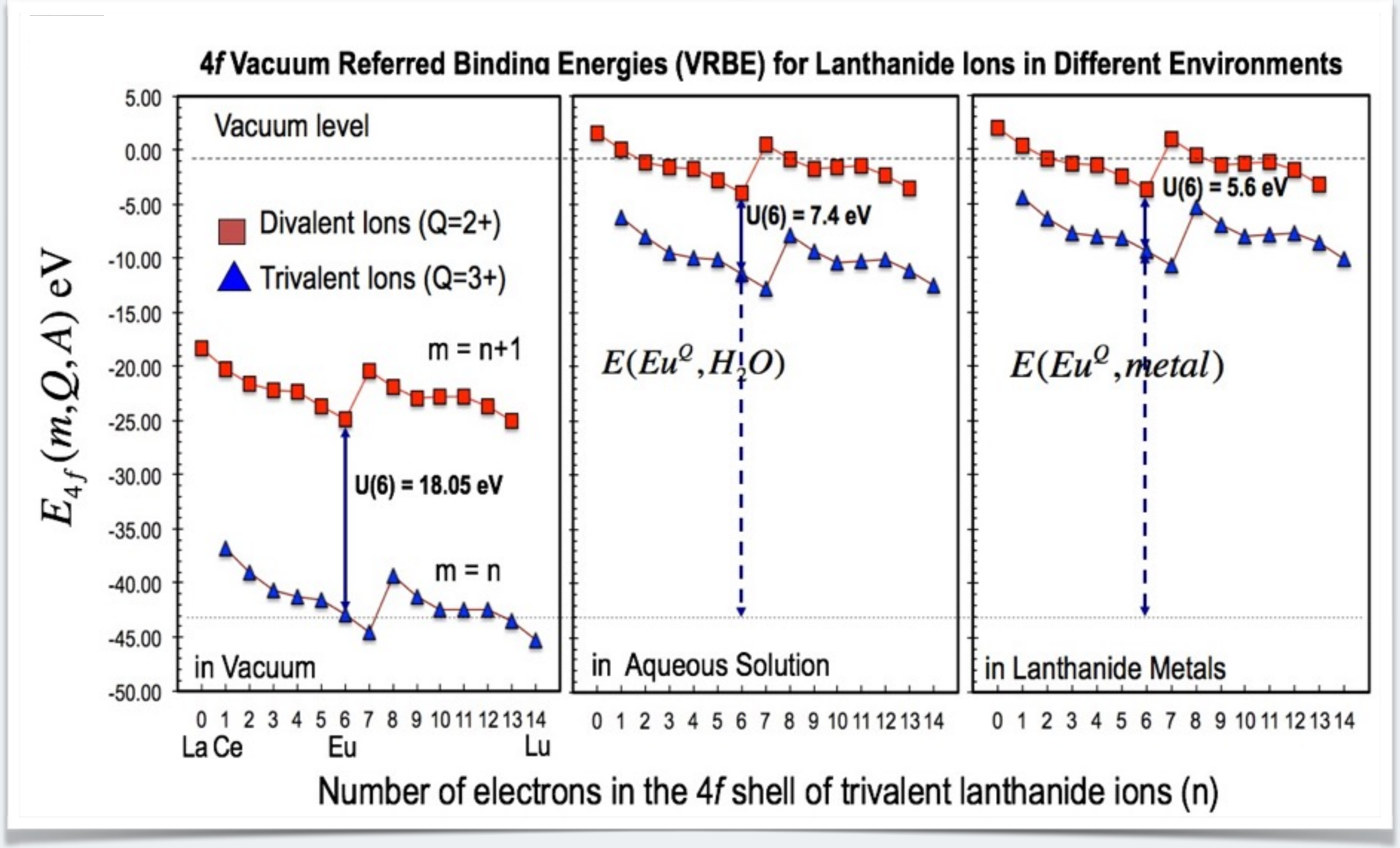
Scintillator Performance
Light output, decay time, radiation tolerance, mechanical strength, attenuation length…

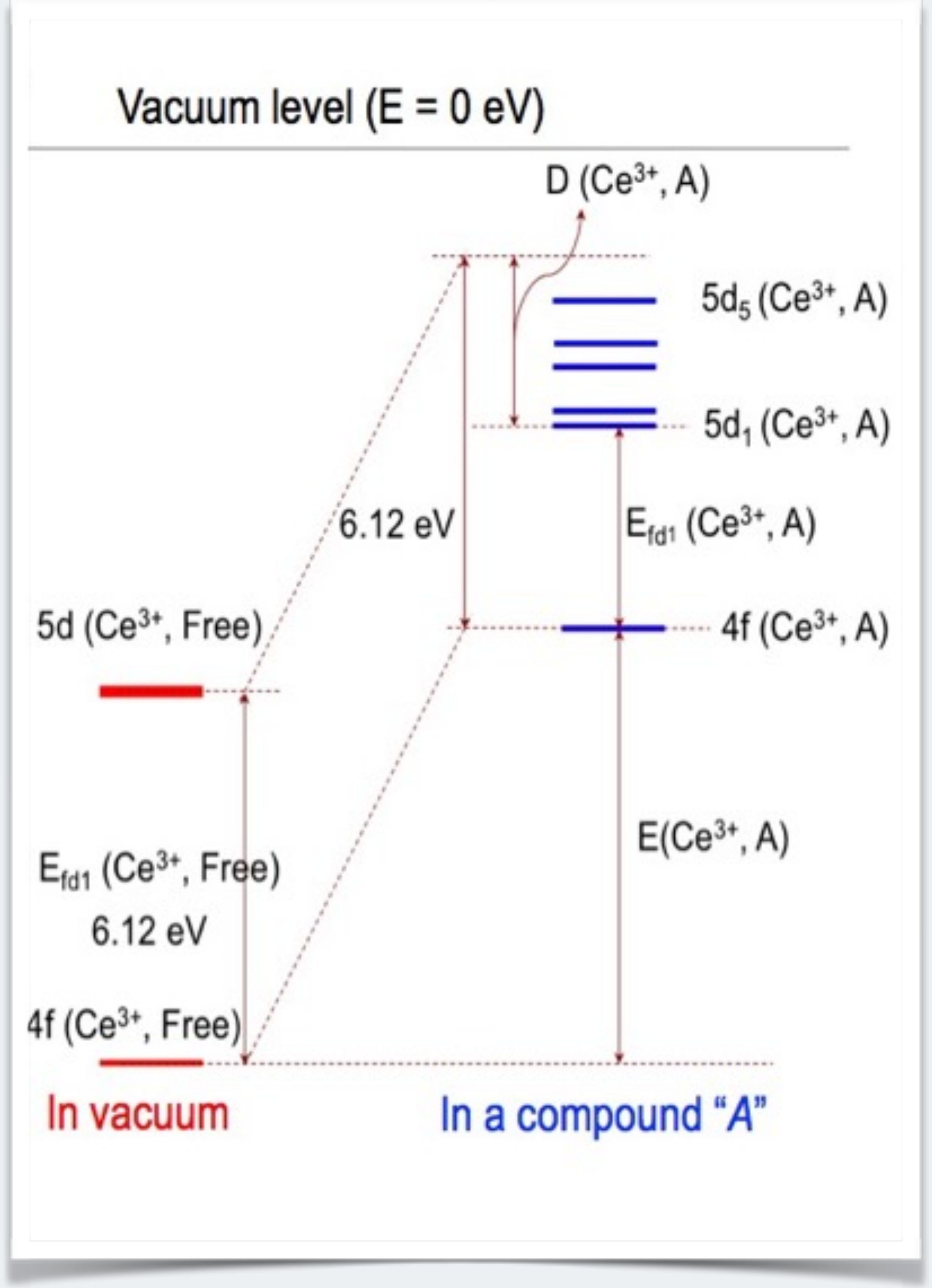
Electronic Structure
Band gap, band dispersion, dielectric screening, activator levels, trap states, phonons…

- Electronic structure directly dictates the scintillator performance portfolio
- In Ln-doped inorganic scintillator chemistries, position of the activator levels with respect to the band edges can be used for a high throughput screening.



Putting the Right Physics in the ML Models





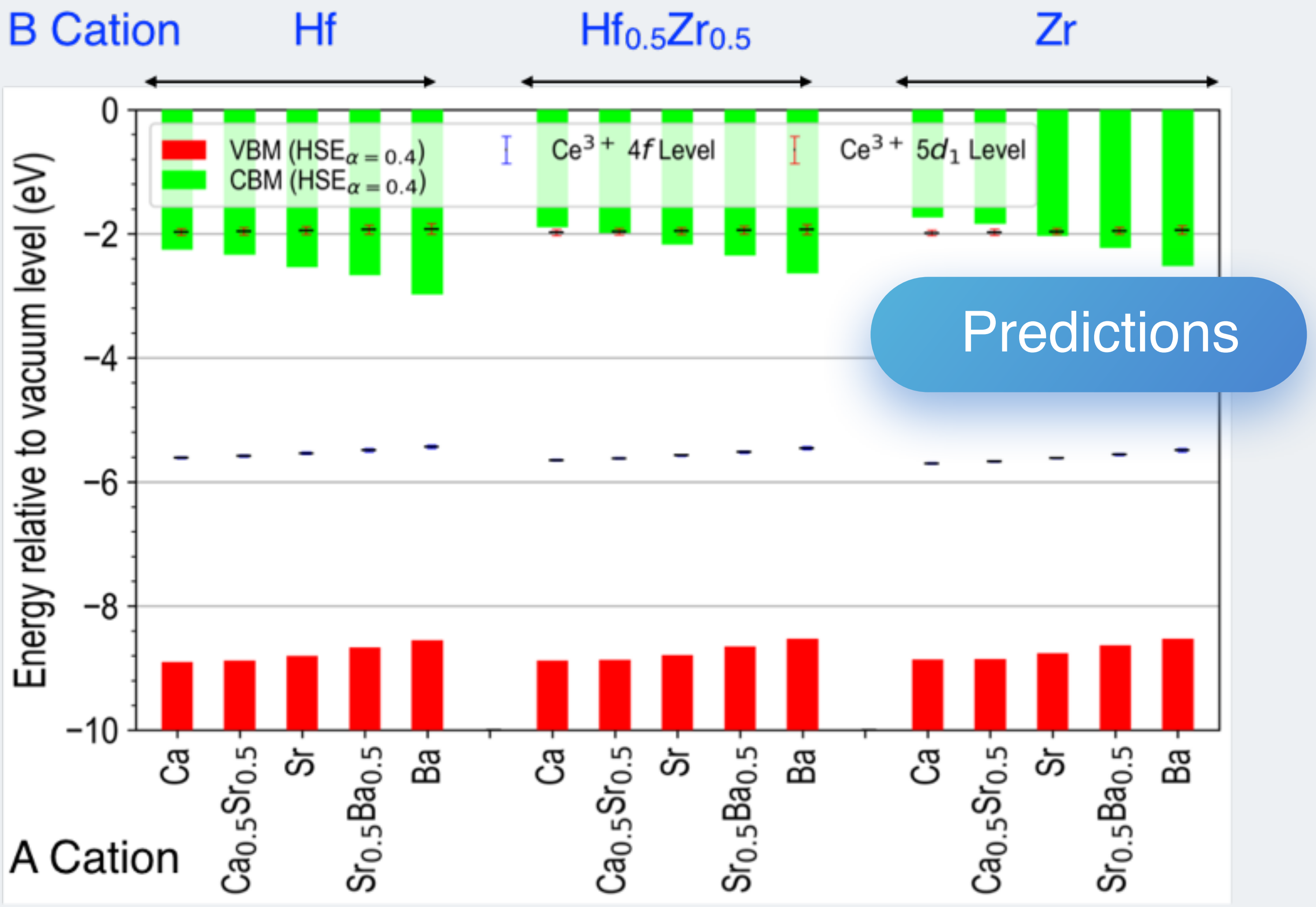
- The "U" parameter is a measure of f shell e-e repulsion in the lanthanide activator
- The "D" parameter is primarily governed by crystal field around the dopant

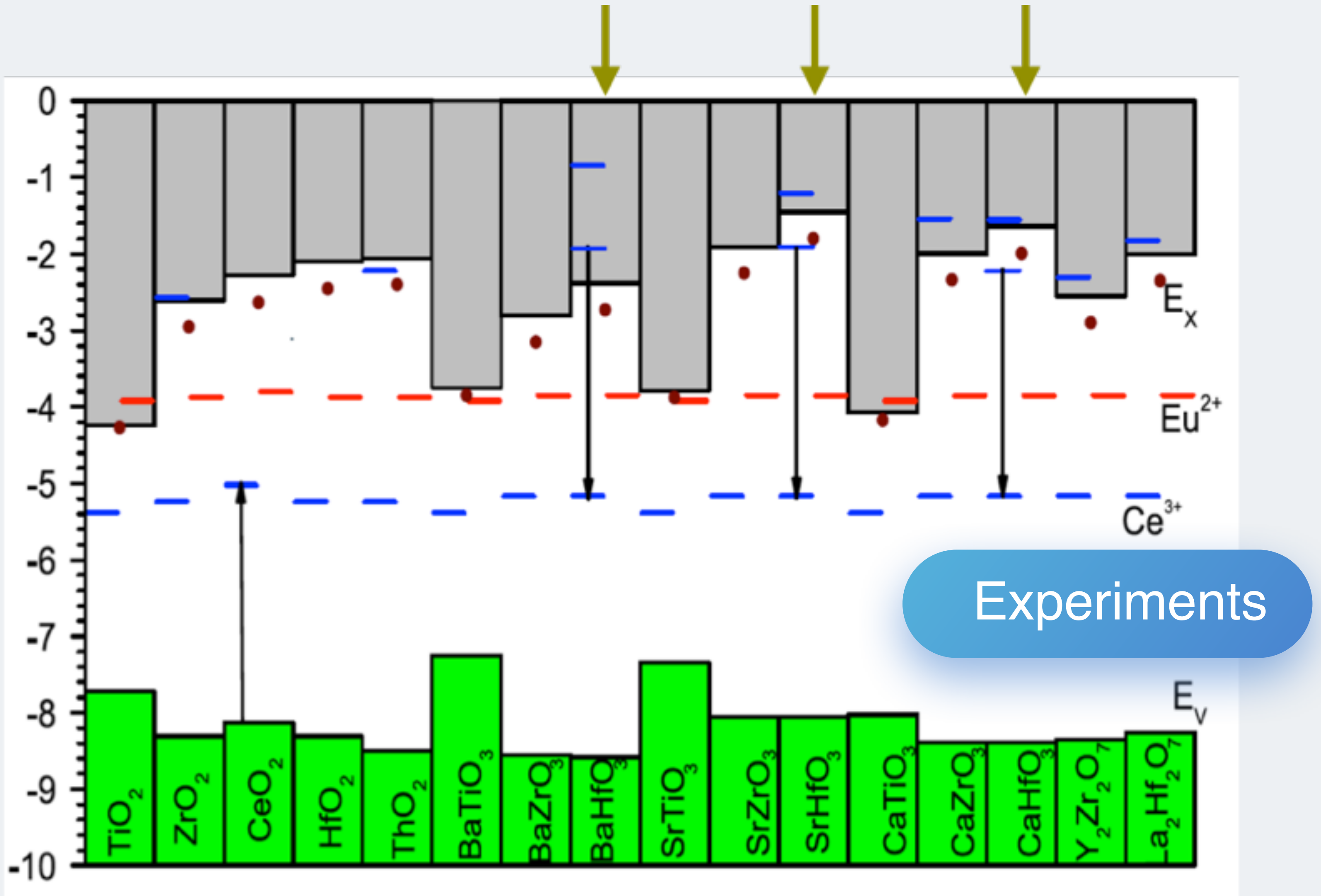
- A knowledge of the "U" and "D" parameters combined with Dorenbos' chemical shift model‡ and DFT-based electronic structure computations for the bandgap allows for an accurate prediction of the 4f and $5d_1$ levels of a lanthanide activator in a given host chemistry.

‡P. Dorenbos, Physical Review B 85, 165107 (2012).

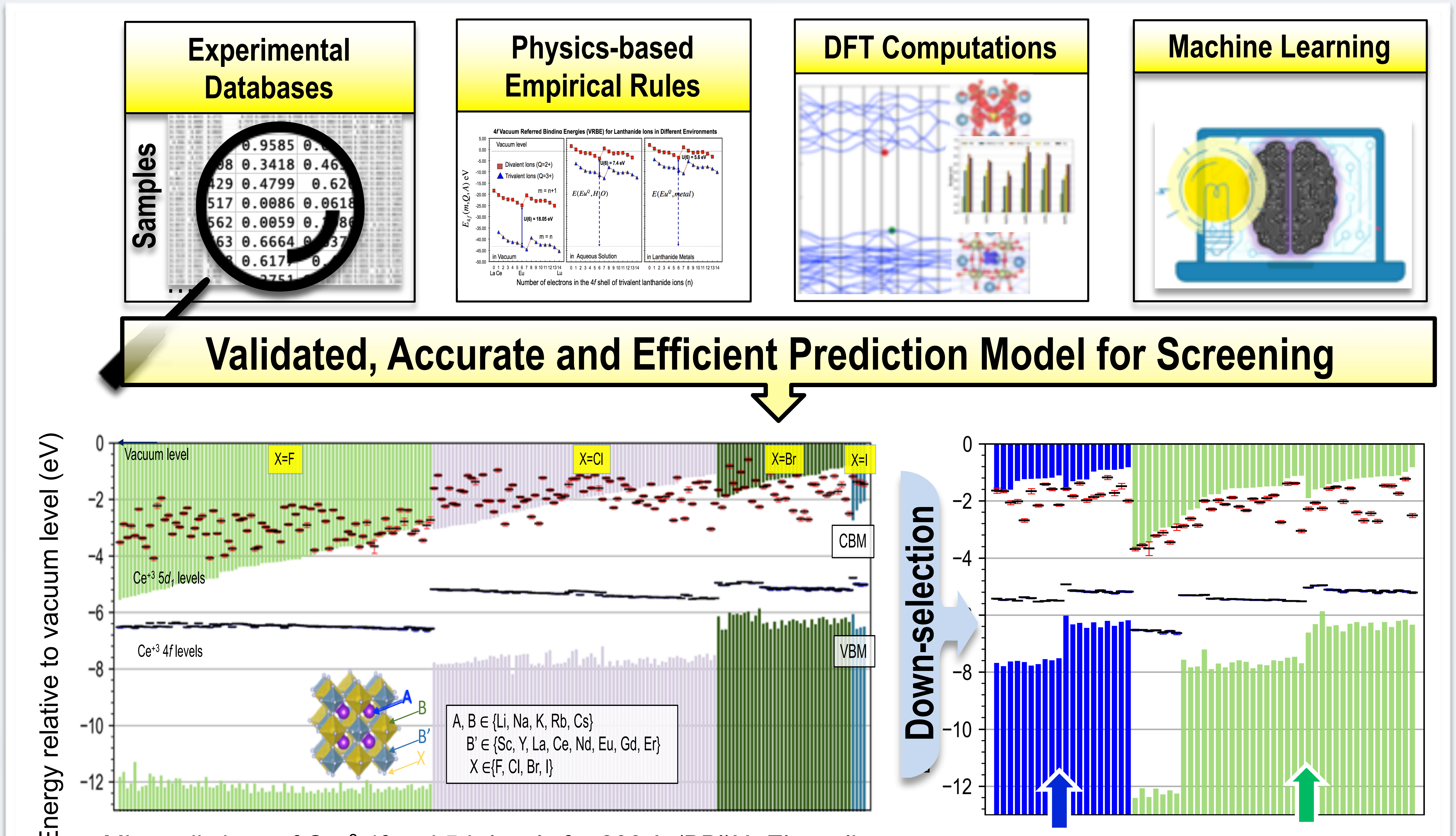
Applications to Perovskites and Elpasolites

Chemical Trends





High Throughput Screening



ML predictions of Ce^{+3} 4f and $5d_1$ levels for 200 $A_2(BB')X_6$ Elpasolites

G. Pilania, S. K. Yadav, M. Nikl, B. P. Uberuaga, and C. R. Stanek, Phys. Rev. Appl. accepted (2018).
G. Pilania, K. Mcclellan, C. R. Stanek and B. P. Uberuaga, J. Chem. Phys. 148, 241729 (2018).